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Quantum fluctuations and kinetic correlation in the strongly Interacting Limit of Density Functional Theory

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KINETIC ENERGY OPERATOR AT DIFFERENT ORDERS

We include here more terms in the expansion of the Laplace-Beltrami operator in somewhat a more detailed fashion than in [14] to show the contribution to dynamics of the two different variables (\mathbf{s}, \mathbf{q}) . We also add the expression for term constant in λ which has not been derived before¹.

First, some definitions. In this appendix the notation will slightly change with respect to the main body of the thesis, as the notation becomes extremely chaotic very quickly.

The indexes $\alpha, \beta, \gamma, \dots$ will denote the derivatives w.r.t. the Cartesian coordinates s ; the indexes μ, ν, \dots will denote the normal coordinates. The latin letter will denote general indexes. When needed, we shall (ab)use of Einstein' summation notation. As a warm-up, we write the metric tensor, \mathfrak{g}

$$\mathfrak{g}_{\alpha\beta} = \frac{\partial \underline{r}}{\partial s_\alpha} \cdot \frac{\partial \underline{r}}{\partial s_\beta} \quad (\text{A.1a})$$

$$\mathfrak{g}_{\alpha\mu} = \sum_{\nu=d+1}^{dN} q_\nu \frac{\partial \underline{e}^\nu(\mathbf{s})}{\partial s_\alpha} \cdot \underline{e}^\mu(\mathbf{s}) \quad (\text{A.1b})$$

$$\mathfrak{g}_{\mu\nu} = \delta_{\mu\nu}. \quad (\text{A.1c})$$

The last line follows from the orthonormality of the local normal modes. It is helpful to denote the normal mode independent part of \mathfrak{g}_{ij} separately

$$\mathfrak{g}_{\alpha\beta} := \frac{\partial \underline{f}(\mathbf{s})}{\partial s_\alpha} \cdot \frac{\partial \underline{f}(\mathbf{s})}{\partial s_\beta} \quad (\text{A.2a})$$

$$g := \det \mathfrak{g}, \quad (\text{A.2b})$$

and to define the tensors Δ and \mathbf{Z} :

$$\Delta_{\alpha\beta}^\mu = -2\underline{e}^\mu(\mathbf{s}) \cdot \frac{\partial^2 \underline{f}(\mathbf{s})}{\partial s_\alpha \partial s_\beta} \quad (\text{A.3a})$$

$$\Delta_{\alpha\nu}^\mu = \underline{e}^\nu(\mathbf{s}) \cdot \frac{\partial \underline{e}^\mu(\mathbf{s})}{\partial s_\alpha} \quad (\text{A.3b})$$

$$\Delta_{\alpha\tau}^\mu = 0 \quad (\text{A.3c})$$

$$\mathbf{Z}_{\alpha\beta}^{\mu\nu} = \frac{\partial \underline{e}^\mu(\mathbf{s})}{\partial s_\alpha} \cdot \frac{\underline{e}^\nu(\mathbf{s})}{\partial s_\beta} \quad (\text{A.3d})$$

$$\mathbf{Z}_{\alpha\nu}^{\mu\nu} = 0 \quad (\text{A.3e})$$

$$\mathbf{Z}_{\nu\tau}^{\mu\nu} = 0. \quad (\text{A.3f})$$

¹ We thank Dr. K. J. H. Giesbertz for helping the author in carrying out and extending the computation of the constant term to general N and d .

Some properties concerning these tensors will turn out helpful in simplifying the steps later, eq. (A.25):

$$\underline{e}^\mu(\mathbf{s}) \cdot \frac{\partial \underline{f}(\mathbf{s})}{\partial s_\alpha} = 0 \Rightarrow \frac{\partial \underline{e}^\mu(\mathbf{s})}{\partial s_\beta} \cdot \frac{\partial \underline{f}(\mathbf{s})}{\partial s_\alpha} + \underline{e}^\mu(\mathbf{s}) \cdot \frac{\partial^2 \underline{f}(\mathbf{s})}{\partial s_\beta \partial s_\alpha} = 0. \quad (\text{A.4})$$

$$\Delta_{\alpha\mu}^\nu + \Delta_{\alpha\nu}^\mu = \underline{e}^\mu(\mathbf{s}) \cdot \frac{\partial \underline{e}^\nu(\mathbf{s})}{\partial s_\alpha} + \underline{e}^\nu(\mathbf{s}) \cdot \frac{\partial \underline{e}^\mu(\mathbf{s})}{\partial s_\alpha} = \frac{\partial}{\partial s_\alpha} \delta_{\mu\nu} = 0 \quad (\text{A.5})$$

With this in mind, the scaled metric tensor reads

$$\begin{pmatrix} \tilde{\mathfrak{G}}_{\alpha\beta} & \tilde{\mathfrak{G}}_{\alpha\gamma} \\ \tilde{\mathfrak{G}}_{\kappa\beta} & \tilde{\mathfrak{G}}_{\kappa\gamma} \end{pmatrix} = \begin{pmatrix} \delta_{\alpha\beta} & 0 \\ 0 & \lambda^{-1/4} \delta_{\kappa\gamma} \end{pmatrix} \cdot \begin{pmatrix} \mathfrak{G}_{\alpha\beta} & \mathfrak{G}_{\alpha\gamma} \\ \mathfrak{G}_{\kappa\beta} & \mathfrak{G}_{\kappa\gamma} \end{pmatrix} \cdot \begin{pmatrix} \delta_{\alpha\beta} & 0 \\ 0 & \lambda^{-1/4} \delta_{\kappa\gamma} \end{pmatrix} \quad (\text{A.6})$$

The general form of the expansion (3.44) reads then

$$\tilde{\mathfrak{G}}_{ik} = \tilde{\mathfrak{G}}_{ik}^0 + \underbrace{\lambda^{-1/4} \sum_{\mu=d+1}^{dN} u_\mu \Delta_{ik}^\mu + \lambda^{-1/2} \sum_{\mu,\nu=d+1}^{dN} u_\mu u_\nu \mathbf{Z}_{ik}^{\mu\nu}}_{:=\mathbb{A}_{ik}}. \quad (\text{A.7})$$

Component by component, this means

$$\begin{aligned} \tilde{\mathfrak{G}}_{\alpha\beta} &= \mathfrak{G}_{\alpha\beta} - \lambda^{-1/4} \sum_{\mu=d+1}^{dN} u_\mu \left(2 \underline{e}^\mu(\mathbf{s}) \cdot \frac{\partial^2 \underline{f}(\mathbf{s})}{\partial s_\alpha \partial s_\beta} \right) \\ &\quad + \lambda^{-1/2} \sum_{\mu,\nu=d+1}^{dN} u_\mu u_\nu \left(\frac{\partial \underline{e}^\mu(\mathbf{s})}{\partial s_\alpha} \cdot \frac{\underline{e}^\nu(\mathbf{s})}{\partial s_\beta} \right) \end{aligned} \quad (\text{A.8})$$

$$\tilde{\mathfrak{G}}_{\alpha\nu} = \lambda^{-1/4} \sum_{\mu=d+1}^{dN} u_\mu \frac{\partial \underline{e}^\mu(\mathbf{s})}{\partial s_\alpha} \cdot \underline{e}^\nu(\mathbf{s}) \quad (\text{A.9})$$

$$\tilde{\mathfrak{G}}_{\mu\nu} = \lambda^{-1/2} \delta_{\mu\nu} \quad (\text{A.10})$$

It is instructive to keep in mind the structure of all the tensors by "representing" them by block matrices:

$$\tilde{\mathfrak{G}}_{ik}^0 = \left(\begin{array}{c|c} \mathfrak{G}_{\alpha\beta} & \mathbb{0} \\ \hline \mathbb{0} & \lambda^{-1/2} \mathbb{1} \end{array} \right) \quad (\text{A.11})$$

$$\Delta^\mu = \left(\begin{array}{c|c} \Delta_{\alpha\beta}^\mu & \Delta_{\alpha\nu}^\mu \\ \hline \Delta_{\alpha\tau}^\mu & \mathbb{0} \end{array} \right) \quad (\text{A.12})$$

$$\mathbf{Z}^{\mu\nu} = \left(\begin{array}{c|c} \mathbf{Z}_{\alpha\beta}^{\mu\nu} & \mathbb{0} \\ \hline \mathbb{0} & \mathbb{0} \end{array} \right) \quad (\text{A.13})$$

All the blocks are matrices of dimensions either $d \times d$ or $d(N-1) \times d(N-1)$ or $d \times d(N-1)$ or $d(N-1) \times d$. It is also clear now that the indexes (α, β) refer to the small squared matrices, the indexes (μ, ν) to the big ones and the indexes (α, μ) and the indexes (μ, α) to the horizontal and vertical rectangular matrices respectively.

Next, we are going to use again

$$\det(\mathbb{X} + \mathbb{A}) = \det(\mathbb{X}) \det(\mathbb{1} + \mathbb{A}\mathbb{X}^{-1}) \quad (\text{A.14})$$

with $\mathbb{X} = \mathbb{g}^0_{ik}$. This implies computing, defining² $(\tilde{\mathbb{g}}^0)^{-1}_{ik} := (\tilde{\mathbb{g}}^{0,ik})$

$$\left(\mathbb{A}(\tilde{\mathbb{g}}^0)^{-1} \right)_{ik} = \lambda^{-1/4} u_\mu \underbrace{\Delta_{ij}^\mu \tilde{\mathbb{g}}^{0,jk}}_{:= \hat{\Delta}_{ik}^\mu} + \lambda^{-1/2} u_\mu u_\nu \underbrace{\mathbb{Z}_{ij}^{\mu\nu} \tilde{\mathbb{g}}^{0,jk}}_{:= \hat{\mathbb{Z}}_{ik}^{\mu\nu}} \quad (\text{A.15})$$

Now we need to use the fact that

$$\begin{aligned} \det(\mathbb{1} + \mathbb{B}) &= \sum_{k=0}^{\infty} \frac{1}{k!} \left(- \sum_{j=1}^{\infty} \frac{(-1)^j}{j} \text{Tr}(\mathbb{B}^j) \right)^k \\ &\approx 1 + \text{Tr}(\mathbb{B}) - \frac{1}{2} \text{Tr}(\mathbb{B}^2) + \frac{1}{2} \text{Tr}(\mathbb{B})^2. \end{aligned} \quad (\text{A.16})$$

We need to compute therefore the trace of $\mathbb{A} (\mathbb{g}^0)^{-1}$ and $\mathbb{A} (\mathbb{g}^0)^{-1} \mathbb{A} (\mathbb{g}^0)^{-1}$. First however simplify the computation by noticing that to leading order

$$\mathbb{A} (\mathbb{g}^0)^{-1} \mathbb{A} (\mathbb{g}^0)^{-1} \sim \lambda^{-1/2} u_\mu u_\nu \hat{\Delta}^\mu \cdot \hat{\Delta}^\nu, \quad (\text{A.17})$$

implying

$$\begin{aligned} &\det \left(\mathbb{1} + \mathbb{A} (\tilde{\mathbb{g}}^0)^{-1} \right) \\ &= 1 + \lambda^{-1/4} u_\mu \text{Tr} (\hat{\Delta}^\mu) + \lambda^{-1/2} u_\mu u_\nu \left(\text{Tr} (\hat{\mathbb{Z}}^{\mu\nu}) - \frac{1}{2} \text{Tr} (\hat{\Delta}^\mu \hat{\Delta}^\nu) + \frac{1}{2} \text{Tr} (\hat{\Delta}^\mu) \text{Tr} (\hat{\Delta}^\nu) \right). \end{aligned} \quad (\text{A.18})$$

We arrive finally at

$$\begin{aligned} &\det(\tilde{\mathbb{g}}) \\ &= g \left[1 + \lambda^{-1/4} u_\mu \text{Tr} (\hat{\Delta}^\mu) + \lambda^{-1/2} u_\mu u_\nu \left[\text{Tr} (\hat{\mathbb{Z}}^{\mu\nu}) + \frac{1}{2} (\text{Tr} (\hat{\Delta}^\mu) \text{Tr} (\hat{\Delta}^\nu) - \text{Tr} (\hat{\Delta}^\mu \hat{\Delta}^\nu)) \right] \right]. \end{aligned} \quad (\text{A.19})$$

To proceed, use that

$$\sqrt{1 + \epsilon l + \epsilon^2 m} \approx 1 + \frac{\epsilon}{2} l + \frac{\epsilon^2}{2} \left(m - \frac{l^2}{4} \right) \quad (\text{A.20})$$

² Here we start using Einstein's notation: in each term in which two or more indexes are repeated, a sum symbol is assumed. The sum indexes run over the dimension of the block matrices just showed in (A.11) and following, consistently with the greek letters chosen. We shall not instead make distinctions between covariant and contravariant indexes, unless explicitly specified.

to obtain

$$\begin{aligned} & \sqrt{\det(\tilde{\mathfrak{g}})} \\ & \sim \sqrt{g} \left[1 + \frac{\lambda^{-1/4}}{2} u_\mu \text{Tr}(\hat{\Delta}^\mu) \right. \\ & \quad \left. + \frac{\lambda^{-1/2}}{4} [u_\mu u_\nu \left(2\text{Tr}(\hat{\mathbf{Z}}^{\mu\nu}) + \frac{1}{2} \text{Tr}(\hat{\Delta}^\mu) \text{Tr}(\hat{\Delta}^\nu) \right) - \text{Tr}(\hat{\Delta}^\mu \hat{\Delta}^\nu)] \right]; \end{aligned} \quad (\text{A.21})$$

$$\begin{aligned} & \frac{1}{\sqrt{\det(\tilde{\mathfrak{g}})}} \\ & \sim \frac{1}{\sqrt{g}} \left[1 - \frac{\lambda^{-1/4}}{2} u_\mu \text{Tr}(\hat{\Delta}^\mu) \right. \\ & \quad \left. + \frac{\lambda^{-1/2}}{4} [u_\mu u_\nu \left(-2\text{Tr}(\hat{\mathbf{Z}}^{\mu\nu}) + \frac{1}{2} \text{Tr}(\hat{\Delta}^\mu) \text{Tr}(\hat{\Delta}^\nu) \right) + \text{Tr}(\hat{\Delta}^\mu \hat{\Delta}^\nu)] \right]. \end{aligned} \quad (\text{A.22})$$

The last ingredient we need is the inverse tensor, which can be obtained imposing that $\tilde{\mathfrak{g}}\tilde{\mathfrak{g}}^{-1} = \mathbb{1}$ up to order $\lambda^{-1/2}$. So we write

$$\begin{aligned} \tilde{\mathfrak{g}}^{-1} & \sim (\tilde{\mathfrak{g}}^0)^{-1} - \lambda^{-1/4} (\tilde{\mathfrak{g}}^0)^{-1} \\ & \quad \times \left[u_\mu \hat{\Delta}^\mu + \lambda^{-1/2} u_\mu u_\nu \left(\mathbf{Z}^{\mu\nu} - \hat{\Delta}^\mu (\tilde{\mathfrak{g}}^0)^{-1} \hat{\Delta}^\nu \right) \right] (\tilde{\mathfrak{g}}^0)^{-1}. \end{aligned} \quad (\text{A.23})$$

Now we have all the ingredient to compute the Laplace Beltrami operator, which reads

$$\hat{T} = \sqrt{\lambda} \left(-\frac{1}{2} \sum_{\mu=d+1}^{dN} \frac{\partial^2}{\partial u_\mu^2} \right) + \lambda^{1/4} \left(-\frac{1}{4} \sum_{\mu=d+1}^{dN} \text{Tr}(\hat{\Delta}^\mu) \frac{\partial}{\partial u_\mu} \right) + \hat{T}^{(\infty)}. \quad (\text{A.24})$$

The operator $\hat{T}^{(\infty)}$ has an involved expression and does not fit in one line:

$$\begin{aligned} -2\hat{T}^{(\infty)} & = \mathfrak{g}^{\alpha\beta} \frac{\partial^2}{\partial s_\alpha \partial s_\beta} + \left(\frac{\mathfrak{g}^{\alpha\beta}}{2g} \frac{\partial g}{\partial s_\beta} + \frac{\partial \mathfrak{g}^{\alpha\beta}}{\partial s_\beta} \right) \frac{\partial}{\partial s_\beta} - 2u_\mu \hat{\Delta}_{\tau\alpha} \frac{\partial^2}{\partial s_\alpha \partial u_\tau} - \\ & \quad \left(\frac{\hat{\Delta}_{\tau\alpha}^\mu}{2g} \frac{\partial g}{\partial s_\alpha} + \frac{\partial \hat{\Delta}_{\tau\alpha}^\mu}{\partial s_\alpha} + u_\mu \left(\frac{1}{2} \text{Tr}(\hat{\Delta}^\mu \hat{\Delta}^\tau) - \text{Tr}(\hat{\mathbf{Z}}^{\mu\tau}) - \hat{\Delta}_{\nu\alpha}^\mu \hat{\Delta}_{\alpha\tau}^\mu \right) \right) \frac{\partial}{\partial u_\tau} \\ & \quad + u_\mu u_\nu \hat{\Delta}_{\tau\alpha}^\mu \hat{\Delta}_{\alpha\sigma}^\nu \frac{\partial^2}{\partial u_\tau \partial u_\sigma}. \end{aligned} \quad (\text{A.25})$$

As complicated as it can look like, for $N = 2$, $d = 1$ the Laplace Beltrami operator reduces to a quite simple form:

$$\begin{aligned} \nabla^2 & \sim \left[\sqrt{\lambda} \frac{\partial^2}{\partial^2 u} - \lambda^{1/4} \frac{f''}{(1+f'^2)^{3/2}} \frac{\partial}{\partial u} \right. \\ & \quad \left. + \left(\frac{3f'f''}{(1+f'^2)^2} \frac{\partial}{\partial s} - \frac{uf''^2}{(1+f'^2)^3} \frac{\partial}{\partial u} + \frac{1}{1+f'^2} \frac{\partial^2}{\partial s^2} \right) \right]. \end{aligned} \quad (\text{A.26})$$

CO-MOTION FUNCTIONS FOR THE ANALYTICAL DENSITIES

$q_1(x)$ Let's consider $q_1(x) = \frac{\text{sech}(x)}{2 \arctan(\tanh(5))}$. From eq. (4.2) we have:

$$\begin{aligned} N_e(s) &\equiv \int_{-10}^s \frac{\text{sech}(x)}{2 \arctan[\tanh(5)]} dx = \\ &= 1 + \frac{\arctan \left[\tanh \left(\frac{s}{2} \right) \right]}{\arctan [\tanh(5)]} \\ N_e^{-1}(s) &= 2 \operatorname{arctanh} [\tan [(x-1) \arctan [\tanh(5)]]] \end{aligned} \quad (\text{B.1})$$

and using eq. (5.1) we find

$$f[q_1](s) = 2 \operatorname{arctanh} \left(\tan \left(\frac{1}{2} (\operatorname{gd}(s) - \operatorname{sign}(s) \operatorname{gd}(10)) \right) \right), \quad (\text{B.2})$$

$\operatorname{gd}(s)$ being the Gudermannian function.

$q_2(x)$ Let's consider $q_2(x) = \frac{1}{(1+x^2) \arctan(10)}$. From eq. (4.2) we have:

$$\begin{aligned} N_e(s) &\equiv \int_{-10}^s \frac{1}{(1+x^2) \arctan(10)} dx = \\ &= 1 + \frac{\arctan(s)}{\arctan(10)} \\ N_e^{-1}(s) &= \tan [(s-1) \arctan(10)] \end{aligned} \quad (\text{B.3})$$

and using eq. (5.1) we find

$$f[q_2](s) = \tan \left[\arctan(10) \left[\frac{\arctan(s)}{\arctan(10)} - \operatorname{sign}(s) \right] \right]. \quad (\text{B.4})$$

CALCULATION DETAILS FOR $\delta F^{\text{ZPE}} / \delta \varrho(x)$

We have from (5.5)

$$\frac{\delta F^{\text{ZPE}}[\varrho]}{\delta \varrho(x)} = \frac{\omega(x)}{4} + \frac{1}{4} \int_{-\infty}^{\infty} dy \varrho(y) \frac{\delta \omega(y)}{\delta \varrho(x)}. \quad (\text{C.1})$$

Using the chain rule in (5.8), the integral in the last equation can be written as

$$\begin{aligned} \int_{-\infty}^{\infty} dy \varrho(y) \frac{\delta \omega(y)}{\delta \varrho(x)} &= \int_{-\infty}^{\infty} dy \frac{\omega(y)}{2} \frac{f'(y)^2 - 1}{f'(y)^2 + 1} (\delta(y - x) - f'(y) \delta(f(y) - x)) \\ &\quad + \int_{-\infty}^{\infty} dy \frac{\omega(y)}{2} \left(\frac{v_{ee}'''(f(y) - y)}{v_{ee}''(f(y) - y)} - \frac{f'(y)^2 - 1}{f'(y)^2 + 1} \frac{\varrho'(f(y))}{\varrho(f(y))} \right) \\ &\quad \cdot f'(y) (\Theta(y - x) - \Theta(f(y) - x)). \end{aligned} \quad (\text{C.2})$$

With the substitution $u = f(y)$, the second delta function and step function can be combined with the first ones to yield

$$\begin{aligned} \int_{-\infty}^{\infty} dy \varrho(y) \frac{\delta \omega(y)}{\delta \varrho(x)} &= \int_{-\infty}^{\infty} dy \omega(y) \frac{f'(y)^2 - 1}{f'(y)^2 + 1} \delta(y - x) \\ &\quad + \int_{-\infty}^{\infty} dy \frac{\omega(y)}{2} \left[\frac{v_{ee}'''(f(y) - y)}{v_{ee}''(f(y) - y)} (f'(y) + 1) - \frac{f'(y)^2 - 1}{f'(y)^2 + 1} \left(f'(y) \frac{\varrho'(f(y))}{\varrho(f(y))} + \frac{\varrho'(y)}{\varrho(y)} \right) \right]. \end{aligned} \quad (\text{C.3})$$

The integrand of last integral is not well behaved due to the presence of $\omega(y)$, and is prone to numerical instabilities when evaluated. In our investigation we found that both integrals have opposite divergences, which can be eliminated by combining them. In order to do so, we proceed along two lines: first, we integrate the Dirac deltas in the first term and then rewrite the result as an integral, effectively performing an integration by parts of the Dirac delta. Secondly, remembering that the functional derivative is only defined modulo a constant, we can shift the region of integration, as this only gives a constant contribution and write

$$\begin{aligned} \int_{-\infty}^{\infty} dy \varrho(y) \frac{\delta \omega(y)}{\delta \varrho(x)} &= \omega(x) \frac{f'(x)^2 - 1}{f'(x)^2 + 1} \\ &\quad + \int_x^{b_+} dy \frac{\omega(y)}{2} \left[\frac{v_{ee}'''(f(y) - y)}{v_{ee}''(f(y) - y)} (f'(y) + 1) \right. \\ &\quad \left. - \frac{f'(y)^2 - 1}{f'(y)^2 + 1} \left(f'(y) \frac{\varrho'(f(y))}{\varrho(f(y))} + \frac{\varrho'(y)}{\varrho(y)} \right) \right], \end{aligned} \quad (\text{C.4})$$

where we defined $b_+ > 0$ as the point where $b_+ = -f(b_+)$. As outlined, we can now use the fundamental theorem of calculus to rewrite the first term as

$$\omega(x) \frac{f'(x)^2 - 1}{f'(x)^2 + 1} = \int_{b_+}^x dy \left(\omega'(y) \frac{f'(y)^2 - 1}{f'(y)^2 + 1} + \frac{4\omega(y)}{(f'(y) + 1/f'(y))^2} \frac{f''(y)}{f'(y)} \right). \quad (\text{C.5})$$

We make use of

$$\begin{aligned} \omega'(y) &= \frac{1}{2\omega(y)} \left[v_{ee}'''(f(y) - y)(f'(y) - 1) \left(f'(y) + \frac{1}{f'(y)} \right) \right. \\ &\quad \left. + v_{ee}''(f(y) - y) \left(1 - \frac{1}{f'(y)^2} \right) f''(y) \right], \end{aligned} \quad (\text{C.6a})$$

$$f''(y) = f'(y) \left(\frac{\varrho'(y)}{\varrho(y)} - f'(y) \frac{\varrho'(f(y))}{\varrho(f(y))} \right) \quad (\text{C.6b})$$

to write

$$\begin{aligned} \omega(x) \frac{f'(x)^2 - 1}{f'(x)^2 + 1} &= \int_{b_+}^x dy \left[\frac{v_{ee}'''(f(y) - y)}{2\omega(y)} (f'(y) - 1) (f'(y) - f'(y)^{-1}) \right. \\ &\quad \left. + \frac{v_{ee}''(f(y) - y)}{2\omega(y)} \frac{f'^2(y) + f'(y)^{-2} + 6}{f'(y) + f'(y)^{-1}} \left(\frac{\varrho'(y)}{\varrho(y)} - f'(y) \frac{\varrho'(f(y))}{\varrho(f(y))} \right) \right]. \end{aligned} \quad (\text{C.7})$$

Combining these results we can write the integral in (C.1) as

$$\begin{aligned} \int_{-\infty}^{\infty} dy \varrho(y) \frac{\delta \omega(y)}{\delta \varrho(x)} &= \int_x^{b_+} dy \left[v_{ee}'''(f(y) - y) \frac{f'(y) + 1}{\omega(y)} \right. \\ &\quad \left. - \frac{v_{ee}''(f(y) - y)}{\omega(y)} \left(\frac{\varrho'(y)}{\varrho(y)} \frac{f'(y)^2 + 3}{f'(y) + f'(y)^{-1}} - f'(y) \frac{\varrho'(f(y))}{\varrho(f(y))} \frac{f'(y)^{-2} + 3}{f'(y) + f'(y)^{-1}} \right) \right]. \end{aligned} \quad (\text{C.8})$$

It is not transparent from this expression that (C.8) is odd under the exchange $x \rightarrow f(x)$. Moreover, the term $\sim v_{ee}''' f / \omega$ might not be bounded. To make it more clear, we apply again the transformation $u = f(y)$ to the first two terms in the integrand above and rewrite them as

$$\begin{aligned} &\int_x^{b_+} dy \left[v_{ee}'''(f(y) - y) \frac{f'(y)}{\omega(y)} - \frac{v_{ee}''(f(y) - y)}{\omega(y)} \frac{\varrho'(y)}{\varrho(y)} \frac{f'(y)^2 + 3}{f'(y) + f'(y)^{-1}} \right] \\ &= - \int_{f(x)}^{-b_+} du \left[\frac{v_{ee}'''(f(u) - u)}{\omega(u)} \right. \\ &\quad \left. + \frac{v_{ee}''(f(u) - u)}{\omega(u)} f'(u) \frac{\varrho'(f(u))}{\varrho(f(u))} \frac{f'(u)^{-2} + 3}{f'(u) + f'(u)^{-1}} \right]. \end{aligned} \quad (\text{C.9})$$

Now the integrands can be summed to yield

$$\begin{aligned}
 & \int_{-\infty}^{\infty} dy \varrho(y) \frac{\delta \omega(y)}{\delta \varrho(x)} \\
 &= \left(\int_x^{b_+} dy + \int_{-b_+}^{f(x)} dy \right) \\
 & \times \left[\frac{v_{ee}'''(f(y) - y)}{\omega(y)} + \frac{v_{ee}''(f(y) - y)}{\omega(y)} \frac{\varrho'(f(y))}{\varrho(f(y))} \frac{3f'(y) + f'(y)^{-1}}{f'(y) + f'(y)^{-1}} \right],
 \end{aligned} \tag{C.10}$$

and adding the integration between $-b_+$ and b_+ , which amounts to adding only an immaterial constant to the functional derivative, yields (5.12).

LDA FOR ELECTRONS IN 1D

For electrons in 1D with the interaction given by eq. (7.17), the exchange energy is known analytically,

$$\epsilon_x(\varrho) = -\frac{1}{2} \varrho g(b\pi \varrho), \quad (\text{D.1})$$

with the function

$$g(z) = \frac{1}{2z^2} \left\{ -\gamma + \exp(z^2) \text{Ei}(-z^2) - 2 \ln z + G_{2,3}^{2,2} \left(z^2 \middle| \begin{matrix} 1, \frac{3}{2} \\ 1, 1, 2 \end{matrix} \right) \right\}. \quad (\text{D.2})$$

Here, $\gamma = -0.577216$ is Euler's constant, $\text{Ei}(u) = -\mathcal{P} \int_{-u}^{\infty} \frac{e^{-t}}{t} dt$ is the exponential integral function, and G denotes the Meijer G function. As the analytical $g(z)$ is numerically unstable, we expand $g(z) = g_{<}(z) + \mathcal{O}(z^{14})$ for small z and $g(z) = g_{>}(z) + \mathcal{O}(z^{-16})$ for large z ,

$$g_{<}(z) = \sum_{m=0}^7 \left[a_m - b_m \log(z) \right] z^{2m}, \quad (\text{D.3a})$$

$$g_{>}(z) = \frac{\pi^{3/2}}{2z} - \frac{\log(z)}{z^2} + \sum_{m=0}^7 c_m z^{-2m}. \quad (\text{D.3b})$$

As the minimum difference $|g_{<}(z) - g_{>}(z)|$, occuring at $z = z_0 \approx 1.68$, is extremely small, we simply truncate the two expansions, to obtain the approximation

$$g(z) \approx \tilde{g}(z) \equiv \begin{cases} g_{<}(z) & z \leq z_0, \\ g_{>}(z) & z > z_0. \end{cases} \quad (\text{D.4})$$

Notice the small discontinuity of $\tilde{g}(z)$ at z_0 in Fig. D.1. The coefficients a_m, b_m, c_m of Eq. D.3 are listed in Table D.2.

For the correlation energy, we use the parametrization from Ref. [167],

$$\epsilon_c(r_s) = -\frac{1}{2} \frac{r_s}{A + Br_s^n + Cr_s^2} \ln(1 + \alpha r_s + \beta r_s^m), \quad (\text{D.5})$$

with the 1D density parameter $r_s = \frac{1}{2\varrho}$.

The values of the 7 parameters $A, B, C, n, \alpha, \beta, m$ are different for different values of b , see Table IV of Ref. [167]. For convenience of the reader, we report them in Table D.1.

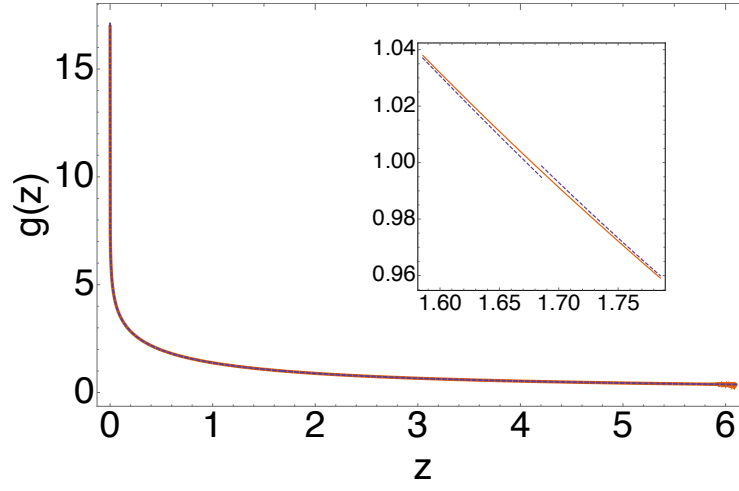


Figure D.1: Comparison between $g(z)$ (red, solid) and $\tilde{g}(z)$ (violet, dashed). The two curves are almost on top. Moreover, $\tilde{g}(z)$ is still evaluated exactly at large arguments, while $g(z)$ shows numerical instability already at $z \sim 6$.

Table D.1: The set of parameters used in eq. (D.5) for $b = 0.1$ in the interaction (7.17)

A	B	C	α	β	n	m
4.66	2.092	3.735	23.63	109.9	1.379	1.837

Table D.2: List of coefficients used in eq. (D.3)

	$m = 0$	$m = 1$	$m = 2$	$m = 3$
a_m	1.21139	0.132454	0.0276020	0.00533283
b_m	1.00000	0.166667	0.0333333	0.00595238
c_m	0	-1.2886100	-0.16666667	0.1
	$m = 4$	$m = 5$	$m = 6$	$m = 7$
a_m	0.000892750	0.0001297100	0.0000165559	0
b_m	0.000126263	0.0000152625	0	0
c_m	-0.142857	0.3333333333	-1.09090909091	4.61538

CODE TO PRODUCE N COMOTION FUNCTIONS

The following code has been written using the programming language MATLAB[®]. Follows a plot showing the outcome for $N = 20$

```
Ne=dx*cumsum(dens); % dens is the
    density
Ajminval=1:(NumPart-1); %NumPart is the number of
    particles
parfor j15=1:(NumPart-1)
    [minval,HOLD]=min(abs(Ne-j15*UN0));
    Ajminval(j15)=HOLD;
end
fnum=zeros(Nx,NumPart); %Nx is the number of
    gridpoints
tempf=ones(Nx,1);
fnum(:,NumPart)=x;
for j16=fliplr(1:length(Ajminval))
    parfor j14=1:Nx
        if j14<=Ajminval(j16)
            [mincom,xcom]=min(abs(Ne-(Ne(j14)+(NumPart+1-j16)-1)
                *UN0)); %UN0 is a vector
                of 1s
        else
            [mincom,xcom]=min(abs(Ne-(Ne(j14)+(NumPart+1-j16)-1-
                NumPart)*UN0));
        end
        tempf(j14)=x(xcom);
    end
    fnum(:,j16)=tempf;
    clear tempf;
end
```

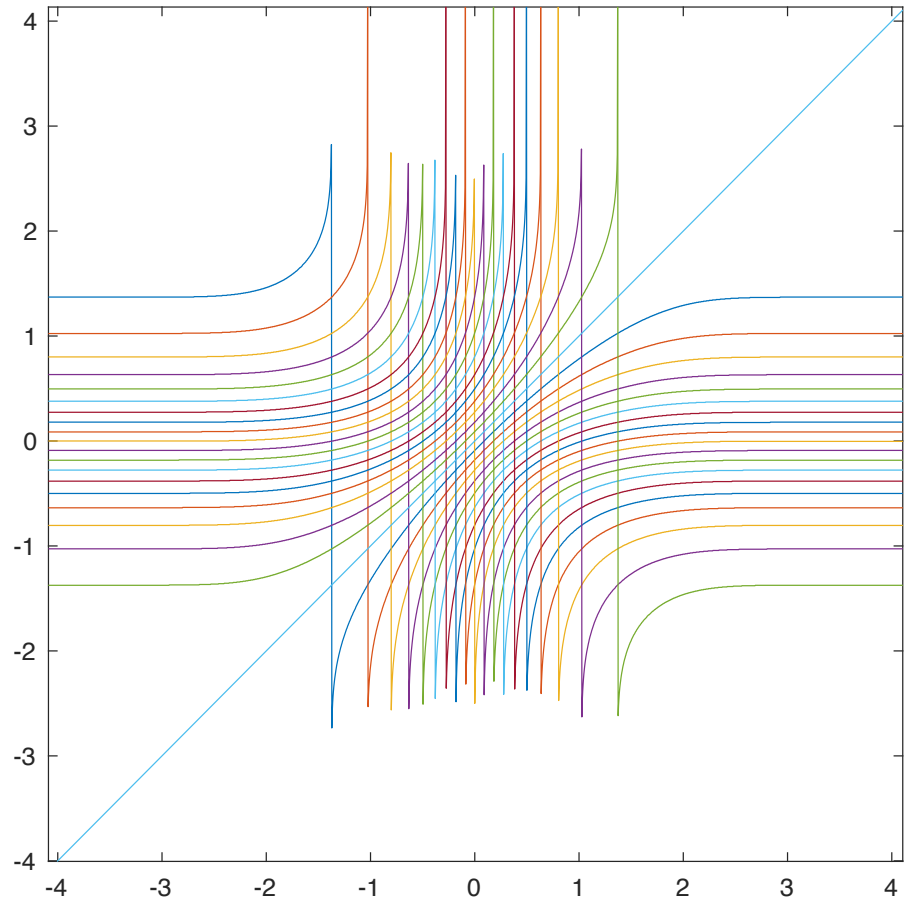


Figure E.1: $N = 20$ comotion function for the density $\tilde{\rho}$ normalized via a proper choice of the prefactor \mathcal{N} .

ASYMPTOTIC EXPANSION OF THE EXCHANGE OPERATOR

Consider a $dN \times dN$ matrix \mathbb{A} . Assume \mathbb{A} is real, symmetric, positive definite. Define $\underline{r} \equiv (\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N) \in \mathbb{R}^{dN}$. Assume a set of N distinct points \mathbf{u}_i , collected in \underline{u} , is given. Consider

$$\Psi_{\alpha(\lambda)}(\underline{r}) = \left(\frac{\alpha(\lambda)^{Nd} \det(\mathbb{A})}{(2\pi)^{Nd}} \right)^{\frac{1}{4}} e^{-\frac{\alpha(\lambda)}{2} (\underline{r}-\underline{u})^T \cdot \mathbb{A} \cdot (\underline{r}-\underline{u})} \quad (\text{F.1})$$

In what follows we consider the term only the term $i = 1$ from eq. (8.6) Let's partition the matrix \mathbb{A} according to

$$\mathbb{A} = \left(\begin{array}{c|ccc} \sigma_1 & & \beta & \\ \hline & \dots & \dots & \dots \\ \beta^T & \dots & \delta & \dots \\ & \dots & \dots & \dots \end{array} \right) \quad (\text{F.2})$$

where σ_1 and γ are real symmetric matrices of dimension d and $(N-1)d$ respectively. We can carry on the integration over $\{\mathbf{r}_2, \dots, \mathbf{r}_N\}$ and compute γ_1 :

$$\begin{aligned} \gamma_1(\mathbf{r}, \mathbf{r}') &= \left(\frac{\alpha(\lambda)^{Nd} \det(\mathbb{A})}{(2\pi)^{Nd}} \frac{(2\pi)^{d(N-1)}}{\alpha(\lambda)^{d(N-1)} \det(\delta)} \right)^{\frac{1}{2}} \\ &\cdot e^{\frac{\alpha(\lambda)}{2} (\beta^T(\mathbf{r}+\mathbf{r}'-2\mathbf{u}_1))^T \delta^{-1} (\beta^T(\mathbf{r}+\mathbf{r}'-2\mathbf{u}_1))} e^{-\frac{\alpha(\lambda)}{2} ((\mathbf{r}-\mathbf{u}_1)^T \sigma_1 (\mathbf{r}-\mathbf{u}_1) + (\mathbf{r}'-\mathbf{u}_1)^T \sigma_1 (\mathbf{r}'-\mathbf{u}_1))} \\ &= \left(\frac{\det(\mathbb{A}) \alpha(\lambda)^d}{(2\pi)^d \det(\delta)} \right)^{\frac{1}{2}} \\ &\cdot e^{-\frac{\alpha(\lambda)}{2} ((\mathbf{r}-\mathbf{u}_1)^T \sigma_1 (\mathbf{r}-\mathbf{u}_1) + (\mathbf{r}'-\mathbf{u}_1)^T \sigma_1 (\mathbf{r}'-\mathbf{u}_1) + \frac{\alpha(\lambda)}{2} (\mathbf{r}+\mathbf{r}'-2\mathbf{u}_1)^T \underbrace{\beta \delta^{-1} \beta^T}_{=\zeta} (\mathbf{r}+\mathbf{r}'-2\mathbf{u}_1))} \\ &\cdot e \end{aligned} \quad (\text{F.3})$$

Assume $\alpha(\lambda)$ is a monotonically increasing function of a positive real parameter λ . We are interested in the asymptotic behaviour at large λ of

$$\begin{aligned} \int \hat{v}(\mathbf{r}, \mathbf{r}') \gamma_1(\mathbf{r}, \mathbf{r}') &= \left(\frac{\det(\mathbb{A}) \alpha(\lambda)^d}{(2\pi)^d \det(\delta)} \right)^{\frac{1}{2}} \sum_{j=1}^{N/2} \int_{\mathbb{R}^d \times \mathbb{R}^d} d\mathbf{t} d\mathbf{t}' \frac{1}{|\mathbf{t} - \mathbf{t}'|} \\ &\cdot e^{-\frac{\alpha(\lambda)}{2} (\mathbf{t}^T \sigma_1 \mathbf{t} + \mathbf{t}'^T \sigma_1 \mathbf{t}') + \frac{\alpha(\lambda)}{2} (\mathbf{t}+\mathbf{t}')^T \zeta (\mathbf{t}+\mathbf{t}')} \phi_j^*(\mathbf{t} + \mathbf{u}_1) \phi_j(\mathbf{t}' + \mathbf{u}_1) \end{aligned} \quad (\text{F.4})$$

The Gaussians are peaked on $\mathbf{0}$, hence we expand the HF orbitals and approximate F.4 as

$$\begin{aligned} \int \hat{v}(\mathbf{r}, \mathbf{r}') \gamma_1(\mathbf{r}, \mathbf{r}') &\approx \left(\frac{\det(\mathbb{A}) \alpha(\lambda)^d}{(2\pi)^d \det(\delta)} \right)^{\frac{1}{2}} \underbrace{\sum_j |\phi_j(\mathbf{u}_1)|^2}_{= \frac{Q_{HF}(\mathbf{u}_1)}{2}} \\ &\cdot \int_{\mathbb{R}^d \times \mathbb{R}^d} d\mathbf{r} d\mathbf{r}' \frac{e^{-\frac{\alpha(\lambda)}{2} (\mathbf{t}^T \sigma_1 \mathbf{t} + \mathbf{t}'^T \sigma_1 \mathbf{t}') + \frac{\alpha(\lambda)}{2} (\mathbf{t} + \mathbf{t}')^T \zeta (\mathbf{t} + \mathbf{t}')}}{|\mathbf{t} - \mathbf{t}'|} \end{aligned} \quad (\text{F.5})$$

Scale the coordinates: $\mathbf{t} \mapsto \frac{\mathbf{q}}{\sqrt{\alpha(\lambda)}}$, $\mathbf{t}' \mapsto \frac{\mathbf{q}'}{\sqrt{\alpha(\lambda)}}$ to get

$$\begin{aligned} \int \hat{v}(\mathbf{r}, \mathbf{r}') \gamma_1(\mathbf{r}, \mathbf{r}') &\approx \left(\frac{\det(\mathbb{A}) \alpha(\lambda)^d}{(2\pi)^d \det(\delta)} \right)^{\frac{1}{2}} \alpha(\lambda)^{\frac{1}{2}-d} \frac{Q_{HF}(\mathbf{u}_1)}{2} \\ &\cdot \int_{\mathbb{R}^d \times \mathbb{R}^d} d\mathbf{q} d\mathbf{q}' \frac{e^{-\frac{1}{2} (\mathbf{q}^T \sigma_1 \mathbf{q} + \mathbf{q}'^T \sigma_1 \mathbf{q}') + \frac{1}{2} (\mathbf{q} + \mathbf{q}')^T \zeta (\mathbf{q} + \mathbf{q}')}}{|\mathbf{q} - \mathbf{q}'|} \\ &= \underbrace{\left(\frac{\det(\mathbb{A})}{(2\pi)^d \det(\delta)} \right)^{\frac{1}{2}} \alpha(\lambda)^{\frac{1-d}{2}} \frac{Q_{HF}(\mathbf{u}_1)}{2}}_{=f(\lambda)} \\ &\cdot \int_{\mathbb{R}^d \times \mathbb{R}^d} d\mathbf{q} d\mathbf{q}' \frac{e^{-\frac{1}{2} (\mathbf{q}^T \sigma_1 \mathbf{q} + \mathbf{q}'^T \sigma_1 \mathbf{q}') + \frac{1}{2} (\mathbf{q} + \mathbf{q}')^T \zeta (\mathbf{q} + \mathbf{q}')}}{|\mathbf{q} - \mathbf{q}'|} \end{aligned} \quad (\text{F.6})$$

Next, we do a rotation of the coordinates according to:

$$\frac{\mathbf{q} - \mathbf{q}'}{\sqrt{2}} = \vec{\tau} \quad (\text{F.7})$$

$$\frac{\mathbf{q} + \mathbf{q}'}{\sqrt{2}} = \vec{\mathbf{T}} \quad (\text{F.8})$$

$$\frac{\vec{\mathbf{T}} + \vec{\tau}}{\sqrt{2}} = \mathbf{q} \quad (\text{F.9})$$

$$\frac{\vec{\mathbf{T}} - \vec{\tau}}{\sqrt{2}} = \mathbf{q}' \quad (\text{F.10})$$

$$\int \hat{v}(\mathbf{r}, \mathbf{r}') \gamma_1(\mathbf{r}, \mathbf{r}') \approx \sqrt{2} f(\lambda) \int_{\mathbb{R}^d \times \mathbb{R}^d} d\vec{\mathbf{T}} d\vec{\tau} \frac{e^{-\frac{1}{2} (\vec{\tau}^T \sigma_1 \vec{\tau} + \vec{\mathbf{T}}^T (\sigma_1 + \zeta) \vec{\mathbf{T}})}}{|\vec{\tau}|} \quad (\text{F.11})$$

The integral in $\vec{\mathbf{T}}$ is readily computed and leads to

$$\int \hat{v}(\mathbf{r}, \mathbf{r}') \gamma_1(\mathbf{r}, \mathbf{r}') \approx \sqrt{2} \alpha(\lambda)^{\frac{1-d}{2}} \frac{Q_{HF}(\mathbf{u}_1)}{2} \int_{\mathbb{R}^d} d\vec{\tau} \frac{e^{-\frac{1}{2} (\vec{\tau}^T \sigma_1 \vec{\tau})}}{|\vec{\tau}|} \quad (\text{F.12})$$

where we used the fact that $\det(\mathbb{A}) = \det(\delta) \det(\sigma_1 - \beta^T \delta^{-1} \beta)$. Calling generally σ_i the i -th d distinct dimensional block on the diagonal of \mathbb{A} :

$$\mathbb{A} = \begin{pmatrix} \boxed{\sigma_1} & \dots & \dots \\ \vdots & \boxed{\sigma_2} & \\ \vdots & & \ddots \end{pmatrix} \quad (\text{F.13})$$

we can write

$$\langle \Psi | -\hat{K} | \Psi \rangle_\lambda \approx \sum_{i=1}^N \alpha(\lambda)^{\frac{1-d}{2}} \frac{Q_{HF}(\mathbf{u}_i)}{\sqrt{2}} \int_{\mathbb{R}^d} d\vec{\tau} \frac{e^{-\frac{1}{2}(\vec{\tau}^T \sigma_i \vec{\tau})}}{|\vec{\tau}|} \quad (\text{F.14})$$

We note that the last integral in eq. (F.14) is divergent in $d = 1$, and that an effective Coulomb interaction needs to be used in order to obtain a finite result.

ELECTROSTATIC ENERGY OF A HARTREE PRODUCT OF GAUSSIAN ORBITALS

Take the normalised spherical Gaussian orbitals

$$\phi_i(\mathbf{r}) = \left(\frac{\omega}{\pi}\right)^{\frac{3}{4}} e^{-\frac{\omega}{2}(|\mathbf{r}-\mathbf{u}_i|)^2} \quad (\text{G.1})$$

Assume than each electron is close to one site \mathbf{u} . The "Hartree" wave-function then reads

$$\Psi_H(\mathbf{r}_1, \dots, \mathbf{r}_N) = \prod_{i=1}^N \phi_i(\mathbf{r}_i) \quad (\text{G.2})$$

With this, the expectation value of the electron-electron interaction reads

$$\langle \Psi_H | V_{ee} | \Psi_H \rangle = \frac{1}{2} \frac{\omega^3}{\pi^3} \left(\sum_{i,j} \int d\mathbf{r} d\mathbf{r}' \frac{e^{-\omega|\mathbf{r}-\mathbf{u}_i|^2} e^{-\omega|\mathbf{r}'-\mathbf{u}_j|^2}}{|\mathbf{r}-\mathbf{r}'|} - N \int d\mathbf{r} d\mathbf{r}' \frac{e^{-\omega|\mathbf{r}|^2} e^{-\omega|\mathbf{r}'|^2}}{|\mathbf{r}-\mathbf{r}'|} \right) \quad (\text{G.3})$$

The last integral reads

$$- \frac{1}{2} \frac{\omega^3}{\pi^3} \int d\mathbf{r} d\mathbf{r}' \frac{e^{-\omega|\mathbf{r}|^2} e^{-\omega|\mathbf{r}'|^2}}{|\mathbf{r}-\mathbf{r}'|} = -\sqrt{\frac{\omega}{2\pi}} \quad (\text{G.4})$$

The first integral reads

$$\frac{1}{2} \frac{\omega^3}{\pi^3} \sum_{i,j} \int d\mathbf{r} d\mathbf{r}' \frac{e^{-\omega|\mathbf{r}-\mathbf{u}_i|^2} e^{-\omega|\mathbf{r}'-\mathbf{u}_j|^2}}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{2} \frac{\omega^3}{\pi^3} \sum_{i,j} \left(\frac{\pi}{\omega}\right)^3 \frac{\text{erf}\left(\sqrt{\frac{\omega}{2}}|\mathbf{u}_i - \mathbf{u}_j|\right)}{|\mathbf{u}_i - \mathbf{u}_j|} \quad (\text{G.5})$$

To proceed, rewrite

$$\frac{1}{2} \sum_{i,j} \frac{\text{erf}\left(\sqrt{\frac{\omega}{2}}|\mathbf{u}_i - \mathbf{u}_j|\right)}{|\mathbf{u}_i - \mathbf{u}_j|} = \frac{1}{2} \int_V \sum_i \delta(\mathbf{r} - \mathbf{u}_i) \sum_j \delta(\mathbf{r}' - \mathbf{u}_j) \frac{\text{erf}\left(\sqrt{\frac{\omega}{2}}|\mathbf{r} - \mathbf{r}'|\right)}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}' \quad (\text{G.6})$$

Next, use the definition of reciprocal lattice vector:

$$\sum_i \delta(\mathbf{r} - \mathbf{u}_i) = \frac{1}{V_{cell}} \sum_{\mathbf{G}} e^{-i\mathbf{G} \cdot \mathbf{r}} \quad (\text{G.7})$$

so

$$\frac{1}{2} \sum_{i,j} \frac{\text{erf}\left(\sqrt{\frac{\omega}{2}}|\mathbf{u}_i - \mathbf{u}_j|\right)}{|\mathbf{u}_i - \mathbf{u}_j|} = \frac{1}{2V_{cell}^2} \sum_{\mathbf{G}, \mathbf{G}'} \int_{V_{tot}} e^{-i\mathbf{G} \cdot \mathbf{r}} e^{-i\mathbf{G}' \cdot \mathbf{r}'} f(|\mathbf{r} - \mathbf{r}'|) d\mathbf{r} d\mathbf{r}' \quad (\text{G.8})$$

Now switch to $\mathbf{r} - \mathbf{r}' = \vec{\xi}$, $\mathbf{r} + \mathbf{r}' = 2\mathbf{R}$ to get

$$\begin{aligned} & \frac{1}{2V_{cell}^2} \sum_{\mathbf{G}, \mathbf{G}'} \int_{V_{tot}} e^{-i\mathbf{G} \cdot (\mathbf{R} + \frac{\vec{\xi}}{2})} e^{-i\mathbf{G}' \cdot (\mathbf{R} - \frac{\vec{\xi}}{2})} f(|\vec{\xi}|) d\mathbf{R} d\vec{\xi} \\ &= \frac{1}{2V_{cell}^2} \sum_{\mathbf{G}, \mathbf{G}'} \int_{V_{tot}} d\mathbf{R} d\vec{\xi} f(|\vec{\xi}|) e^{-i(\mathbf{G} + \mathbf{G}') \cdot \mathbf{R}} e^{-i\mathbf{G} \cdot \frac{\vec{\xi}}{2}} e^{i\mathbf{G}' \cdot \frac{\vec{\xi}}{2}} \\ &= \frac{N}{2V_{cell}} \sum_{\mathbf{G}} \int_{V_{tot}} d\vec{\xi} f(|\vec{\xi}|) e^{-i\mathbf{G} \cdot \vec{\xi}} \end{aligned} \quad (\text{G.9})$$

where we used the fact that $V_{tot} = NV_{cell}$ and that

$$\frac{1}{V_{tot}} \int_{V_{tot}} dx e^{-i(\mathbf{q} \cdot \mathbf{x})} = \delta_{\mathbf{q}, \vec{0}} \quad (\text{G.10})$$

Now write

$$\frac{\text{erf}\left(\sqrt{\frac{\omega}{2}}|\vec{\xi}|\right)}{|\vec{\xi}|} = \frac{1}{|\vec{\xi}|} - \frac{\text{erfc}\left(\sqrt{\frac{\omega}{2}}|\vec{\xi}|\right)}{|\vec{\xi}|} \quad (\text{G.11})$$

and use the well-known result that

$$\int_V e^{i\mathbf{k} \cdot \mathbf{r}} \frac{1}{r} d\mathbf{r} = \frac{4\pi}{|\mathbf{k}|^2} \quad (\text{G.12})$$

to get

$$\frac{N}{2V_{cell}} \sum_{\mathbf{G}} \int_{V_{tot}} d\vec{\xi} f(|\vec{\xi}|) e^{-i\mathbf{G} \cdot \vec{\xi}} = \frac{N}{2V_{cell}} \sum_{\mathbf{G}} 4\pi \frac{e^{-\frac{|\mathbf{G}|^2}{2\omega}}}{|\mathbf{G}|^2} \quad (\text{G.13})$$

Subtraction of the Hartree energy and the Hartree potential, yields finally

$$\langle \Psi_H | \hat{V}_{ee} - \hat{J} + U[\varrho] | \Psi_H \rangle = \frac{N2\pi}{V_{cell}} \sum_{\mathbf{G} \neq \vec{0}} \frac{e^{-\frac{|\mathbf{G}|^2}{2\omega}}}{|\mathbf{G}|^2} - N\sqrt{\frac{\omega}{2\pi}} \quad (\text{G.14})$$